dimas Suarez

List of Publications by Year in descending order

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111 papers	3,609 citations	136740 32 h-index	155451 55 g-index
117 all docs	117 docs citations	117 times ranked	4272 citing authors

#	ARTICLE	IF	CITATIONS
1	Amphiphilic cyclodextrins: Dimerization and diazepam binding explored by molecular dynamics simulations. Journal of Molecular Liquids, 2022, 349, 118457.	2.3	6
2	QM/MM Energy Decomposition Using the Interacting Quantum Atoms Approach. Journal of Chemical Information and Modeling, 2022, 62, 1510-1524.	2.5	6
3	Understanding the Conformational Properties of Fluorinated Polypeptides: Molecular Modelling of Unguisin A. Journal of Chemical Information and Modeling, 2021, 61, 223-237.	2.5	2
4	Influence of charge configuration on substrate binding to SARS-CoV-2 main protease. Chemical Communications, 2021, 57, 5314-5317.	2.2	14
5	A Quantum Chemical Topology Picture of Intermolecular Electrostatic Interactions and Charge Penetration Energy. Journal of Chemical Theory and Computation, 2021, 17, 4981-4995.	2.3	7
6	Alkali and Alkalineâ€Earth Cations in Complexes with Small Bioorganic Ligands: Abâ€…Initio Benchmark Calculations and Bond Energy Decomposition. ChemPhysChem, 2020, 21, 99-112.	1.0	10
7	Aptamers targeting protein-specific glycosylation in tumor biomarkers: general selection, characterization and structural modeling. Chemical Science, 2020, 11, 9402-9413.	3.7	22
8	SARS-CoV-2 Main Protease: A Molecular Dynamics Study. Journal of Chemical Information and Modeling, 2020, 60, 5815-5831.	2.5	112
9	Fluorine conformational effects characterized by energy decomposition analysis. Physical Chemistry Chemical Physics, 2019, 21, 25258-25275.	1.3	13
10	Affinity Calculations of Cyclodextrin Hostâ€“Guest Complexes: Assessment of Strengths and Weaknesses of End-Point Free Energy Methods. Journal of Chemical Information and Modeling, 2019, 59, 421-440.	2.5	17
11	Application of the Interacting Quantum Atoms Approach to the S66 and Ionicâ€Hydrogenâ€Bond Datasets for Noncovalent Interactions. ChemPhysChem, 2018, 19, 973-987.	1.0	21
12	Interacting Quantum Atoms Approach and Electrostatic Solvation Energy: Assessing Atomic and Group Solvation Contributions. ChemPhysChem, 2018, 19, 3425-3435.	1.0	5
13	Molecular Dynamics Studies of Matrix Metalloproteases. Methods in Molecular Biology, 2017, 1579, 111-134.	0.4	2
14	Conformational and entropy analyses of extended molecular dynamics simulations of Î±-, Î²- and Î³-cyclodextrins and of the Î²-cyclodextrin/nabumetone complex. Physical Chemistry Chemical Physics, 2017, 19, 1431-1440.	1.3	17
15	Ligand Strain and Entropic Effects on the Binding of Macrocyclic and Linear Inhibitors: Molecular Modeling of Penicillopepsin Complexes. Journal of Chemical Information and Modeling, 2017, 57, 2045-2055.	2.5	7
16	Role of the Protonation State on the Structure and Dynamics of Albumin. Journal of Chemical Theory and Computation, 2016, 12, 1972-1988.	2.3	9
17	Unraveling the distinctive features of hemorrhagic and non-hemorrhagic snake venom metalloproteinases using molecular simulations. Journal of Computer-Aided Molecular Design, 2016, 30, 69-83.	1.3	4
18	Molecular Modeling of Bioorganometallic Compounds: Thermodynamic Properties of Molybdoceneâ€“Glutathione Complexes and Mechanism of Peptide Hydrolysis. ChemPhysChem, 2015, 16, 1646-1656.	1.0	3

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19	Extensive Simulations of the Full-Length Matrix Metalloproteinase-2 Enzyme in a Prereactive Complex with a Collagen Triple-Helical Peptide. Biochemistry, 2015, 54, 1243-1258.	1.2	5
20	Direct methods for computing singleâ€molecule entropies from molecular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 1-26.	6.2	39
21	An Integrated Computational and Experimental Approach to Gaining Selectivity for MMPâ€2 within the Gelatinase Subfamily. ChemBioChem, 2014, 15, 399-412.	1.3	24
22	A combined semiempirical and DFT computational protocol for studying bioorganometallic complexes: Application to molybdoceneâ€“cysteine complexes. Journal of Computational Chemistry, 2014, 35, 324-334.	1.5	3
23	Sampling Assessment for Molecular Simulations Using Conformational Entropy Calculations. Journal of Chemical Theory and Computation, 2014, 10, 4718-4729.	2.3	13
24	Progress towards water-soluble triazole-based selective MMP-2 inhibitors. Organic and Biomolecular Chemistry, 2013, 11, 6623.	1.5	31
25	Insights into the hydrolytic chemistry of molybdocene dichloride based on a theoretical mechanistic study. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	4
26	CENCALC: A computational tool for conformational entropy calculations from molecular simulations. Journal of Computational Chemistry, 2013, 34, 2041-2054.	1.5	32
27	Unraveling the Molecular Structure of the Catalytic Domain of Matrix Metalloproteinase-2 in Complex with a Triple-Helical Peptide by Means of Molecular Dynamics Simulations. Biochemistry, 2013, 52, 8556-8569.	1.2	6
28	Alternative Interdomain Configurations of the Full-Length MMP-2 Enzyme Explored by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 2677-2686.	1.2	8
29	Multibody local approximation: Application to conformational entropy calculations on biomolecules. Journal of Chemical Physics, 2012, 137, 084115.	1.2	22
30	The Basicity of Carbons. , 2012, , 173-203.		12
31	Theoretical Study of the Oxidation of Histidine by Singlet Oxygen. Chemistry - A European Journal, 2012, 18, 8437-8447.	1.7	31
32	Ab Initio Benchmark Calculations on Ca(II) Complexes and Assessment of Density Functional Theory Methodologies. Journal of Physical Chemistry A, 2011, 115, 11331-11343.	1.1	8
33	Entropy Calculations of Single Molecules by Combining the Rigidâ€Rotor and Harmonic-Oscillator Approximations with Conformational Entropy Estimations from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2011, 7, 2638-2653.	2.3	56
34	Quantum chemical calculations of stability constants: study of ligand effects on the relative stability of Pd(II)â€peptide complexes. Theoretical Chemistry Accounts, 2011, 128, 465-475.	0.5	6
35	Ketoneâ€Alcohol Hydrogenâ€Transfer Equilibria: Is the Biooxidation of Halohydrins Blocked?. Chemistry - A European Journal, 2010, 16, 11012-11019.	1.7	46
36	Kinetic and binding effects in peptide substrate selectivity of matrix metalloproteinaseâ€2: Molecular dynamics and QM/MM calculations. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1-11.	1.5	16

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37	Understanding Regioselective Cleavage in Peptide Hydrolysis by a Palladium(II) Aqua Complex: A Theoretical Point of View. Journal of Physical Chemistry B, 2010, 114, 8525-8535.	1.2	11
38	Interdomain Conformations in the Full-Length MMP-2 Enzyme Explored by Proteinâ"Protein Docking Calculations Using pyDock. Journal of Chemical Theory and Computation, 2010, 6, 2204-2213.	2.3	6
39	Molecular dynamics and quantum mechanical calculations on the mononuclear zinc-Î²-lactamase from Bacillus cereus: Protonation state of the active site and imipenem binding. Computational and Theoretical Chemistry, 2009, 912, 105-112.	1.5	2
40	Thermochemical Fragment Energy Method for Biomolecules: Application to a Collagen Model Peptide. Journal of Chemical Theory and Computation, 2009, 5, 1667-1679.	2.3	37
41	Molecular dynamics simulations of the active matrix metalloproteinaseâ€2: Positioning of the Nâ€terminal fragment and binding of a small peptide substrate. Proteins: Structure, Function and Bioinformatics, 2008, 72, 50-61.	1.5	18
42	Peptide Hydrolysis Catalyzed by Matrix Metalloproteinase 2: A Computational Study. Journal of Physical Chemistry B, 2008, 112, 8412-8424.	1.2	32
43	Entropic Control of the Relative Stability of Triple-helical Collagen Peptide Models. Journal of Physical Chemistry B, 2008, 112, 15248-15255.	1.2	17
44	From the X-ray Compact Structure to the Elongated Form of the Full-Length MMP-2 Enzyme in Solution: A Molecular Dynamics Study. Journal of the American Chemical Society, 2008, 130, 14070-14071.	6.6	19
45	Monoligand Zn(II) Complexes:â€‰Ab Initio Benchmark Calculations and Comparison with Density Functional Theory Methodologies. Journal of Chemical Theory and Computation, 2008, 4, 243-256.	2.3	35
46	Molecular Dynamics Simulations of Matrix Metalloproteinase 2:â€‰Role of the Structural Metal Ions[,]. Biochemistry, 2007, 46, 8943-8952.	1.2	37
47	A Computational Study of the Deacylation Mechanism of Human Butyrylcholinesterase. Biochemistry, 2006, 45, 7529-7543.	1.2	22
48	Molecular Dynamics Simulations of Class C Î²-Lactamase fromCitrobacter freundii:Â Insights into the Base Catalyst for Acylationâ€. Biochemistry, 2006, 45, 439-451.	1.2	16
49	Assessing the Protonation State of Drug Molecules:Â The Case of Aztreonam. Journal of Medicinal Chemistry, 2006, 49, 3235-3243.	2.9	13
50	Quantum Chemical Study on the Coordination Environment of the Catalytic Zinc Ion in Matrix Metalloproteinases. Journal of Physical Chemistry B, 2006, 110, 24222-24230.	1.2	19
51	Quantum mechanical and molecular dynamics simulations of ureases and Zn Î²-lactamases. Journal of Computational Chemistry, 2006, 27, 1240-1262.	1.5	55
52	Formation of Trichlorinated Dibenzo-p-dioxins from 2,4-Dichlorophenol and 2,4,5-Trichlorophenolate: A Theoretical Study. ChemPhysChem, 2006, 7, 2331-2338.	1.0	5
53	Theoretical Studies on the Ring Opening of β-lactams: Processes in Solution and in Enzymatic Media. Current Organic Chemistry, 2006, 10, 805-821.	0.9	28
54	Molecular dynamics simulations of human butyrylcholinesterase. Proteins: Structure, Function and Bioinformatics, 2005, 59, 104-117.	1.5	26

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55	Molecular Dynamics Simulations of the TEM-1 Î²-Lactamase Complexed with Cephalothin. Journal of Medicinal Chemistry, 2005, 48, 780-791.	2.9	29
56	Insights into the Base Catalysis Exerted by the DD-Transpeptidase fromStreptomycesK15:Â A Molecular Dynamics Studyâ€. Biochemistry, 2005, 44, 3225-3240.	1.2	5
57	On the nature of basic sites on carbon surfaces: an overview. Carbon, 2004, 42, 1219-1225.	5.4	461
58	PM3-compatible zinc parameters optimized for metalloenzyme active sites. Journal of Computational Chemistry, 2004, 25, 1677-1692.	1.5	32
59	Zn2+catalysed hydrolysis of Î²-lactams: experimental and theoretical studies on the influence of the Î²-lactam structure. New Journal of Chemistry, 2004, 28, 15-25.	1.4	10
60	Conformational properties of penicillins: Quantum chemical calculations and molecular dynamics simulations of benzylpenicillin. Journal of Computational Chemistry, 2003, 24, 1864-1873.	1.5	11
61	A Combined Theoretical and Experimental Research Project into the Aminolysis ofÎ²-Lactam Antibiotics: The Importance of Bifunctional Catalysis. European Journal of Organic Chemistry, 2003, 2003, 4161-4172.	1.2	9
62	Infrared Spectroscopy of Carbon Materials:Â A Quantum Chemical Study of Model Compounds. Journal of Physical Chemistry B, 2003, 107, 6350-6359.	1.2	328
63	Insights into the Acylation Mechanism of Class A Î²-Lactamases from Molecular Dynamics Simulations of the TEM-1 Enzyme Complexed with Benzylpenicillin. Journal of the American Chemical Society, 2003, 125, 672-684.	6.6	61
64	Ureases:â€‰ Quantum Chemical Calculations on Cluster Models. Journal of the American Chemical Society, 2003, 125, 15324-15337.	6.6	82
65	Basic Surface Oxides on Carbon Materials:Â A Global View. Langmuir, 2003, 19, 3505-3511.	1.6	132
66	Insights into the Structure and Dynamics of the Dinuclear Zinc Î²-Lactamase Site fromBacteroides fragilisâ€. Biochemistry, 2002, 41, 6615-6630.	1.2	74
67	Water-Assisted Alkaline Hydrolysis of Monobactams: A Theoretical Study. Chemistry - A European Journal, 2002, 8, 859-867.	1.7	13
68	Theoretical Study of Ammonolysis of Monobactams: Kinetic Role of theN-Sulfonate Group. Helvetica Chimica Acta, 2002, 85, 206-223.	1.0	6
69	Molecular dynamics simulations of the dinuclear zinc-Î²-lactamase from Bacteroides fragilis complexed with imipenem. Journal of Computational Chemistry, 2002, 23, 1587-1600.	1.5	52
70	Molecular Dynamics Study of the IIA Binding Site in Human Serum Albumin:Â Influence of the Protonation State of Lys195 and Lys199. Journal of Medicinal Chemistry, 2001, 44, 250-260.	2.9	74
71	Molecular Dynamics Simulations of the Mononuclear Zinc-Î²-lactamase fromBacillus Cereus. Journal of the American Chemical Society, 2001, 123, 3759-3770.	6.6	75
72	A Theoretical Study of the Aminolysis Reaction of Lysine 199 of Human Serum Albumin with Benzylpenicillin:Â Consequences for Immunochemistry of Penicillins. Journal of the American Chemical Society, 2001, 123, 7574-7583.	6.6	23

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73	Acylation of Class A Î²-lactamases by Penicillins:â€‰ A Theoretical Examination of the Role of Serine 130 and the Î²-lactam Carboxylate Group. Journal of Physical Chemistry B, 2001, 105, 11302-11313.	1.2	42
74	Molecular Dynamics Simulations of the Mononuclear Zinc-Î²-lactamase fromBacilluscereusComplexed with Benzylpenicillin and a Quantum Chemical Study of the Reaction Mechanism. Journal of the American Chemical Society, 2001, 123, 9867-9879.	6.6	66
75	Evaluation of the Catalytic Mechanism of AICAR Transformylase by pH-Dependent Kinetics, Mutagenesis, and Quantum Chemical Calculations. Journal of the American Chemical Society, 2001, 123, 4687-4696.	6.6	15
76	Quantum Chemical Study of Ester Aminolysis Catalyzed by a Single Adenine:Â A Reference Reaction for the Ribosomal Peptide Synthesis. Journal of the American Chemical Society, 2001, 123, 7687-7690.	6.6	16
77	Theoretical Study of Amine-Assisted Aminolysis of Penicillins â^' The Kinetic Role of the Carboxylate Group. European Journal of Organic Chemistry, 2001, 2001, 793-801.	1.2	4
78	New developments in applying quantum mechanics to proteins. Current Opinion in Structural Biology, 2001, 11, 217-223.	2.6	88
79	Pyrone-Like Structures as Novel Oxygen-Based Organic Superbases. Angewandte Chemie - International Edition, 2000, 39, 1320-1323.	7.2	17
80	Hydration of zinc ions: theoretical study of [Zn(H2O)4](H2O)82+ and [Zn(H2O)6](H2O)62+. Chemical Physics Letters, 2000, 326, 288-292.	1.2	45
81	Stereochemistry of the Furanâ^'Maleic Anhydride Cycloaddition:Â A Theoretical Study. Journal of the American Chemical Society, 2000, 122, 390-391.	6.6	37
82	Critical assessment of the performance of the semiempirical divide and conquer method for single point calculations and geometry optimizations of large chemical systems. Journal of Chemical Physics, 2000, 113, 10512-10523.	1.2	45
83	Competition between Hetero-Dielsâ^'Alder and Chelotropic Addition of Sulfur Dioxide. Theoretical and Experimental Substituent Effects on the Relative Stability of 3,6-Dihydro-1,2-oxathiin-2-oxides (Sultines) and 2,5-Dihydrothiophene-1,1-dioxides (Sulfolenes). Anomeric Effects in Sultine and 6-Substituted Derivatives. Journal of Organic Chemistry, 2000, 65, 5075-5076.	1.7	0
84	Theoretical Study of the Water-Assisted Aminolysis of Î²-Lactams:Â Implications for the Reaction between Human Serum Albumin and Penicillins. Journal of the American Chemical Society, 2000, 122, 6710-6719.	6.6	29
85	Zinc Metallo-Î²-Lactamase from Bacteroides fragilis:â€‰ A Quantum Chemical Study on Model Systems of the Active Site. Journal of the American Chemical Society, 2000, 122, 4197-4208.	6.6	84
86	Ammonolysis and Aminolysis ofÎ²-Lactams: A Theoretical Study. Chemistry - A European Journal, 1999, 5, 1045-1054.	1.7	20
87	Theoretical Study of the Ionâ^'Molecule Reaction of the Vinyl Cation with Ethane. Journal of Physical Chemistry A, 1999, 103, 5996-6002.	1.1	10
88	Competition between Wolff Rearrangement and 1,2-Hydrogen Shift in Î²-Oxy-Î±-ketocarbenes:â€‰ Electrostatic and Specific Solvent Effects. Journal of Physical Chemistry B, 1999, 103, 7145-7150.	1.2	7
89	NH3-Assisted Ammonolysis of Î²-Lactams:Â A Theoretical Study. Journal of Organic Chemistry, 1999, 64, 3281-3289.	1.7	16
90	Importance of a Synperiplanar Stepwise Mechanism through Neutral Intermediates in the Aminolysis of Monocyclic Î²-Lactams:Â A Theoretical Analysis. Journal of Organic Chemistry, 1999, 64, 9144-9152.	1.7	11

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91	Contribution of Pyrone-Type Structures to Carbon Basicity:Â An ab Initio Study. Langmuir, 1999, 15, 3897-3904.	1.6	54
92	Theoretical Study of the [2+2] Cycloaddition of Thioketenes with Imines To FormÎ²-Thiolactams. Chemistry - A European Journal, 1998, 4, 328-334.	1.7	9
93	Rearrangement of azirine intermediates to nitriles: Theoretical study of cleavage of 3,4-dihydro-1aH-azirine[2,3-c]pyrrol-2-one to cyanoketene-formaldimine complex. Journal of Computational Chemistry, 1998, 19, 912-922.	1.5	26
94	On the origin of the endo/exo selectivity in Dielsâ€“Alder reactions. Chemical Communications, 1998, , 385-386.	2.2	25
95	Theoretical Study of the Reaction 1[:CH2] + CHO+ â†' CH3+ + CO. Journal of Physical Chemistry A, 1998, 102, 9918-9924.	1.1	6
96	Contribution of the Basal Planes to Carbon Basicity:â€‰ An Ab Initio Study of the H3O+â^Ï€ Interaction in Cluster Models. Journal of Physical Chemistry B, 1998, 102, 5595-5601.	1.2	77
97	Competition between Hetero-Dielsâ^'Alder and Cheletropic Addition of Sulfur Dioxide. Theoretical and Experimental Substituent Effects on the Relative Stability of 3,6-Dihydro-1,2-oxathiin-2-oxides (Sultines) and 2,5-Dihydrothiophene-1,1-dioxides (Sulfolenes). Anomeric Effects in Sultine and 6-Substituted Derivatives. Journal of Organic Chemistry, 1998, 63, 9490-9499.	1.7	21
98	Ab Initio Study of the H2 Elimination from CH2OH+, CH2NH2+, and CH2SH+. Journal of Physical Chemistry A, 1997, 101, 1561-1566.	1.1	21
99	Theoretical Study of the Zwittazido Cleavage of 4-Azido-2-pyrrolinones:Â The Role of Solvent and Substituents. Journal of the American Chemical Society, 1997, 119, 10291-10301.	6.6	15
100	Anomeric Effect in 1,3-Dioxole:Â A Theoretical Study. Journal of the American Chemical Society, 1996, 118, 9850-9854.	6.6	40
101	Ab initio study of the effect of CH ï¿½ï¿½ O hydrogen bonding on theexo/endo stereoselectivity of Diels-Alder reactions of 2-substituted-1,3-dienes with sulfur dioxide. International Journal of Quantum Chemistry, 1996, 57, 493-499.	1.0	7
102	Theoretical Analysis of the Decomposition of Episulfones. The Journal of Physical Chemistry, 1996, 100, 13462-13465.	2.9	16
103	Mechanism of cheletropic reactions of 1,3-dienes with sulfur dioxide. , 1996, 9, 17.		2
104	Theoretical study of the gas-phase addition of HF and HCl to ethylene: Analysis of the catalytic action of dimeric halides. Journal of Computational Chemistry, 1995, 16, 659-666.	1.5	20
105	Hetero-diels-alder additions of sulfur dioxide to 1,3-dienes: a proposal for a new reactive diene from ab initio calculations. Tetrahedron, 1995, 51, 12661-12666.	1.0	4
106	A Comparative Analysis of the Mechanisms of Cheletropic and Diels-Alder Reactions of 1,3-Dienes with Sulfur Dioxide: Kinetic and Thermodynamic Controls. Journal of Organic Chemistry, 1995, 60, 2848-2852.	1.7	39
107	Solvent effects on the stereoselectivity of keteneâ€“imine cycloaddition reactions. Journal of the Chemical Society Chemical Communications, 1995, , 1677-1678.	2.0	14
108	Solvent effects on hetero Dielsâ€“Alder reactions of sulfur dioxide with 1,3-dienes. Journal of the Chemical Society Chemical Communications, 1994, , 1683-1684.	2.0	15

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109	Ab Initio Study of the Thermal and Lewis Acid-Catalyzed Hetero Diels-Alder Reactions of 1,3-Butadiene and Isoprene with Sulfur Dioxide. Journal of Organic Chemistry, 1994, 59, 8058-8064.	1.7	38
110	Ab initio study of the Lewis acid-catalyzed Diels-Alder reaction of sulfur dioxide with isoprene: regioselectivity and stereoselectivity. Journal of the American Chemical Society, 1994, 116, 763-764.	6.6	47
111	ANACAL: a program to carry out a configurational analysis of the wave function of reactive systems. Computer Physics Communications, 1993, 76, 235-249.	3.0	37